NIST/TRC Databases and Software for Chemistry and Engineering

M. Frenkel,[C,S] R.D. Chirico, Q. Dong, X. Yan, X. Hong, R.C. Wilhoit, V.V. Diky
R.A. Stevenson, and G.R. Hardin

Thermodynamics Research Center (TRC)
Physical and Chemical Properties Division
National Institute of Standards and Technology
325 Broadway, Boulder, CO   80305-3328, U.S.A.

NIST/TRC SOURCE was designed and built as an extensive relational data archival system of experimental thermophysical, thermochemical, and transport properties, which have been reported in the world's scientific literature. It has grown extensively in size and functionality during the past 15 years. SOURCE now consists of over 1 million numerical values on 17,000 pure compounds, 11,000 binary and ternary mixtures, and 4000 reaction systems. Stored also in SOURCE are approximately 115,000 records of compound identification and 83,000 records of bibliographic information. By far, this is the largest data depository system worldwide covering data for more than 120 distinct properties.

SOURCE contains estimated uncertainties for practically all of the numerical data stored, which makes SOURCE uniquely positioned to serve as the foundation of dynamic data-evaluation methods. The design of SOURCE is based strictly on the principles of chemical thermodynamics; in particular, the Gibbs phase rule. Currently, SOURCE resides on a DEC alpha-workstation and is managed by an ORACLE database support system.

The NIST/TRC WinTable database is designed to retrieve and display recommended property values of pure compounds in the TRC Table Database. WinTable is essentially the electronic version of the TRC Tables-Hydrocarbons and TRC Tables-Non-Hydrocarbons compiled by TRC for more than 50 years. At present, WinTable includes more than 497,000 property data points and 4,450 sets of equation coefficients for 7,468 compounds and 33 properties.

Other specific property or compound based databases will be demonstrated.

Guided Data Capture software (GDC) has been developed at NIST/TRC for mass-scale abstraction from the literature of experimental thermophysical and thermochemical property data. This software is freely available for download from the Internet. GDC is currently for data submission directly by authors of publications in the Journal of Chemical and Engineering Data. Expansion of this process to other journals is planned. The procedures of GDC use will be demonstrated. GDC is also used to produce ThermoML files. A collection of ThermoML files, representing experimental data reported by the authors, is available for unrestricted access on the Web.